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14. ABSTRACT

This document is the final report for AFOSR Grant F49620-97-1-0172, "Lattice-Gas Models of Complex-Fluid Hydrodynamics." Under the terms of this grant, the Center for Computational Science at Boston University provided theoretical and computational support to the Lattice-Gas Theory and Computation group at the Space Vehicles Directorate of Air Force Research Laboratory (AFOSR task 2304CP). The principal research topics were the development of lattice-gas and lattice Boltzmann models for complex fluids and droplets, the development and analysis of quantum lattice-gas automata, and the development of unconditionally stable entropic lattice Boltzmann models for viscous fluid dynamics. Nine publications have resulted from this effort, as well as the editorship of the Proceedings of the Seventh International Conference on Discrete Models for Fluid Mechanics as a special issue of the *International Journal of Modern Physics C*. The principal results of this work are described and their significance is placed in historical perspective.

15. SUBJECT TERMS

lattice gases, lattice Boltzmann models, hydrodynamics, complex fluids, emulsions, amphiphilic fluids, entropic lattice Boltzmann models, quantum computation

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Contents

1 Historical Background

1.1 Lattice Gases

The first isotropic lattice-gas automata (LGA) for hydrodynamics were introduced in the late 1980's [1, 2, 3]. Such models consist of discrete particles moving and colliding on a lattice, conserving mass and momentum as they do. If the lattice has sufficient symmetry, it can be shown that the density and hydrodynamic velocity of the particles satisfy the Navier-Stokes equations in the appropriate scaling limit.

This method exploits an interesting fact of kinetic theory: The Navier-Stokes equations are the dynamic renormalization group fixed point for the hydrodynamic behavior of a system of particles whose collisions conserve mass and momentum. This is why a wide range of real fluids with dramatically different molecular properties – such as air, water, honey and oil – can all be described by the Navier-Stokes equations. A lattice gas can then be understood as a "minimalist" construction of such a set of interacting particles. Viewed in this way, it is perhaps less surprising that they satisfy the Navier-Stokes equations in the scaling limit.

For a time, lattice-gas models were actively investigated as an alternative methodology for computational fluid dynamics (CFD) [4]. Unlike all prior CFD methodologies, they do not begin with the Navier-Stokes equations; rather, these equations are an *emergent* property of the particulate model. One often overlooked advantage of this approach is the unconditional stability of such algorithms. By insisting that lattice-gas collisions obey a detailed-balance condition, as do real collisions, we are ensured of the validity of Boltzmann's *H* theorem, which provides a Lyapunov function ensuring the stability of the numerical algorithm. More glibly stated, lattice gases avoid numerical instabilities in precisely the same way that Nature herself does so.

In spite of these appealing features, the presence of intrinsic kinetic fluctuations makes lattice-gas models less than ideal as a CFD methodology. Accurate values for the velocity field at selected locations, or even for bulk coefficients such as drag and lift, have an intrinsic statistical error that can be reduced only by extensive averaging. Consequently, many CFD researchers who appreciated the emergent nature of lattice-gas hydrodynamics but wanted to eliminate (or at least control) the level of fluctuations, turned their attention to the direct simulation of the Boltzmann equation for lattice gases; this is the lattice Boltzmann approach, described below. On the other hand, the presence of such fluctuations in a simple hydrodynamic model make lattice gases an ideal tool for studying the statistical physics of fluids, molecular hydrodynamics, and complex-fluid hydrodynamics. Not surprisingly, these remain the method's principal application areas. Thus, lattice-gas models have evolved into a kind of "fast" molecular dynamics (MD). For these reasons, this report will aim to contrast lattice-gas methods with MD, and lattice Boltzmann methods with CFD.

1.2 Lattice Boltzmann Methods

Models that aim to evolve a real-valued single-particle distribution function, rather than the discrete particles themselves, are called *lattice Boltzmann* (LB) models [5]. Such methods eliminate particle discreteness effects, including kinetic noise and fluctuations. Early attempts along these lines restricted attention to Boltzmann equations for actual lattice gases [6]. It was soon realized, however, that these quickly become unwieldy as the number of possible particle velocities increases. In order for lattice Boltzmann models to become practical tools, it was necessary to develop simplified collision operators that did not necessarily correspond to an underlying lattice-gas model. The most successful collision operators of this type are those of the form due to Bhatnager, Gross and Krook [7], and these have given rise to the so-called lattice BGK models [8].

Lattice BGK collision operators allow the user to specify the form of the equilibrium distribution function to which the fluid should relax. For lattice gases obeying a detailed balance [1] condition, this is known to be a Fermi-Dirac distribution. Having abandoned lattice-gas collision operators, however, it seemed unnecessary to continue to use lattice-gas equilibria, and practitioners exploited the freedom of choosing lattice BGK equilibria to achieve certain desiderata, such as Galilean invariance, and the correct form of the compressible Navier-Stokes equations.

The alert reader will have noticed, however, that the evolution to lattice-BGK methods has jettisoned the last vestiges of kinetic-level physics that might have been left over from the original lattice-gas models. The move to a Boltzmann description of the lattice gas eliminated kinetic fluctuations, but at least it retained an

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[1] Actually, a weaker condition called *semi-detailed balance* suffices for this purpose.

H-theorem; that is, its global equilibrium still extremized a Lyapunov function of the dynamics. The move to lattice-BGK operators and the arbitrary legislation of the equilibrium distribution function, however, completely abandoned even the concept of detailed balance and the H-theorem. Without a Lyapunov function, lattice-BGK methods became susceptible to a wide variety of numerical instabilities which are ill-understood and remain the principal obstacle to the wider application of the technique to the present day.

1.3 Quantum Lattice-Gas Automata

From a computational point of view, the distinction between lattice-gas and lattice Boltzmann models can be understood in terms of the requisite data structures. Lattice-gas particles can be represented by discrete bits, reflecting the presence or absence of particles with given locations and momenta. Lattice Boltzmann models require real numbers on the lattice to represent the corresponding values of the single-particle distribution function. It is somewhat of a logical progression then to ask what might be accomplished with a complex-number representation. One answer is provided by work of Meyer [9], and of Boghosian and Taylor [10, 11, 12]: By interpreting the complex quantities as quantum amplitudes, and insisting that their collisions be unitary transformations, it is possible to create a lattice model whose "hydrodynamics" are the Schrödinger equation for a single particle in an arbitrary potential well.

Since the Schrödinger equation for N particles in D dimensions evolves in an ND dimensional configuration space, a lattice of ND dimensions must be used for the corresponding *quantum lattice-gas automaton* (QLGA). This becomes unwieldy very quickly on any classical computer. As shown by Boghosian and Taylor [12], however, a D dimensional array of real unitary scatterers, in which complete quantum coherence is maintained, could in principle be used to perform this computation in the laboratory in a time independent of N. Thus, quantum lattice-gas automata have become a paradigm for *quantum computation*, rather different from other quantum computing paradigms currently under consideration. This paradigm is a direct embodiment of Feynman's observation that a quantum mechanical system is perhaps best simulated by another quantum mechanical system [13].

1.4 Motivation for the Present Work

The preceeding subsections provide the historical context for the collaboration between Boston University and AFRL, under the terms of AFOSR Grant F49620-97-1-0172, "Lattice-Gas Models of Complex-Fluid Hydrodynamics." Lattice-fluid algorithms attracted the attention of the Lattice-Gas Theory and Computation group at the Space Vehicles Directorate of AFRL who initiated AFOSR task 2304CP to study their application to fluids, complex fluids, and quantum computing. The Center for Computational Science at Boston University provided theoretical and computational support to this group for their work on the following three extensions of the lattice-fluid methodology:

- Exploitation of the role of LGA as an accelerated MD to study the hydrodynamics and rheology of complex-fluids and droplets

- Stabilization of LB models by the reintroduction of an H theorem

- Development of QLGA models for advanced simulation of electronic structure and fluid dynamics on quantum computers

This report shall describe the progress made in each of these areas as a result of the collaboration. The presentation is intended to emphasize the motivation and significance of the principal discoveries made.

The escalation of interest in lattice-fluid models has led to a series of successful international meetings on "Discrete Methods of Fluid Mechanics." The seventh such meeting was held in Oxford, England in July, 1998. The proceedings of this meeting were edited by the principal investigator of this grant, and published as a special issue of the *International Journal of Modern Physics C*. The table of contents of this special issue is presented in Appendix C. The next meetings will be in Santa Fe, New Mexico (2000), Cargese, Corsica (2001), and Shanghai (2002).

2 Principal Areas of Study

2.1 Lattice Models for Complex Fluid Dynamics

Complex fluids are those which, owing to chemical makeup and/or thermodynamic properties, exhibit a variety of emergent structures over broad scales of length and time. Examples include polymers, liquid crystals, emulsions and microemulsions, colloids, glasses and granular materials. Emulsions and microemulsions are examples of amphiphilic fluids – they contain a species of amphiphile, or surfactant, whose free energy is lowered when it is on an interface. This effectively arrests the phase separation process, since that tends to reduce interface, and results in stable droplets or extended structures whose interfaces are loaded with amphiphile. There are a great many open questions concerning the dynamics of this arrested phase separation.

Because hydrodynamic equations are often not known for such materials, researchers sometimes resort to molecular dynamics in an effort to elucidate their time-dependent behavior. Such molecular dynamics simulations must evolve on time scales of 10^{-15} seconds, and are therefore not suitable for studying phenomena that develop on much longer mesoscopic and macroscopic time scales. Emulsion droplets, for example, involve the organization of order 3×10^7 molecules on length scales of order 50 nm ($5 \times 10-6$ cm), and time scales of order 10^{-7} seconds. It would thus take on the order of 3×10^{15} molecular dynamics particle pushes to see the formation of a single such droplet. This is marginally possible today, and indeed it has been accomplished for individual micelles using supercomputer facilities [14].

By contrast, lattice fluid models effectively offer a coarse-grained version of molecular dynamics. In particular, lattice-gas particles typically collide on the order of once per time step, and they move one lattice unit between collisions. Thus, a single lattice-gas time step corresponds to about a mean-free time of evolution. Likewise, a single lattice site represents on the order of a cubic mean-free path of fluid. Since it contains order 10 lattice-gas particles, each lattice-gas particle represents approximately 10^{-1} cubic mean-free paths of fluid.

For dense fluids – i.e., liquids – a mean-free time is about 5×10^{-13} seconds; this is about 500 times longer than a single MD time step, but still about 200,000 times smaller than the micelle formation time. Likewise, a mean-free path is a few nanometers long; this is much longer than a single MD step (order 3×10^{-11} cm), but order 10 times smaller than a micelle diameter. A cubic mean-free path then contains something in the vicinity of 4×10^4 particles, so one lattice-gas particle represents about a tenth of this, or 4×10^3 molecules. The total potential computational savings of lattice-gases over MD is thus $(500)(4 \times 10^4) \sim 2 \times 10^6$. Thus, order 2×10^9 lattice-gas particle pushes will be sufficient to form a single micelle, and a 100×100 grid is sufficient to resolve an entire field of micelles. This reduces the problem from one that is marginally tractable on a supercomputer, to one that is easily performed on a workstation.

One of the results of AFOSR grant number F49620-95-1-0285 was a lattice-gas model of amphiphilic fluids in two spatial dimensions. Such fluids consist of two immiscible phases which are made to mix by the addition of a surfactant or amphiphile, and have a wide variety of applications in the Air Force and throughout industry. In a 1996 paper in the *Proceedings of the Royal Society of London* [15], which was written as part of grant number F49620-95-1-0285, we showed how the lattice-gas methodology could be extended to model an amphiphilic fluid. During grant number F49620-97-1-0172, which is the subject of this paper, I am pleased to report that we made substantial progress on this model. Most importantly, we extended it to three spatial dimensions [16], and we developed a lattice Boltzmann version of the model as well [17].

The three dimensional version of the lattice-gas model for amphiphilic fluids was constructed on the three-dimensional projection of the four-dimensional face-centered hypercubic (FCHC) lattice. This lattice is known [3] to yield isotropic Navier-Stokes flow for a single fluid, and has been used as the basis of other multiphase lattice-gas models [18]. Phase space is indexed by a lattice position, and a discrete velocity. The occupation of each such phase-space location is specified by two bits of species information (representing a water molecule, an oil molecule, an amphiphile molecule, or nothing). Phase-space locations with an amphiphile also have an *director* vector, specifying its direction of orientation.

The FCHC lattice has coordination number 24. These directions are augmented by two rest particles, for a total of 26 possible particle velocities at each site. Two bits per direction means that the species occupation is specified by 52 bits per site. That is, each site can be in one of 2^{52} species states. Unlike the
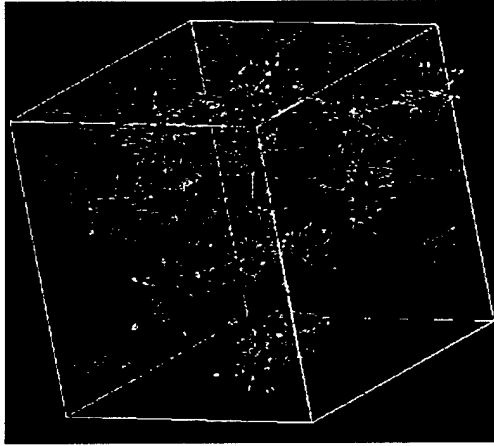
Figure 1: Spherical emulsion droplets in 3D lattice-gas model
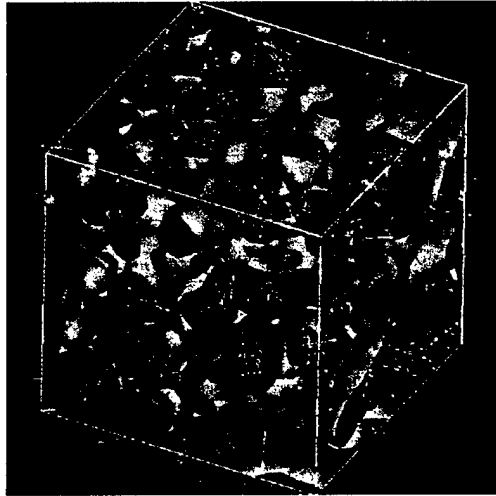

Figure 2: Wormlike micelles in 3D lattice-gas model

two-dimensional version of the model, this number is far too high to make a direct lookup table practical for determining the collision outcomes. Instead, we make use of the fact that there are three subsets of 8 FCHC lattice vectors that lie on the faces of a regular four-dimensional hypercube. We perform sequential collisions on each of these three subsets, each augmented by the two rest particles to allow them to "communicate." It therefore becomes necessary to construct a lookup table for ten velocities; since there are two bits per velocity, the table is indexed by 20 bits, so the number of possible states is 2^{20}, or about 1M. Since the state outcomes are encoded into 4 byte words, the lookup table requires 4 Mbytes of local memory, which is easily within the capability of modern multiprocessors.

The three-dimensional model was shown to exhibit all of the phenomenology of its two-dimensional counterpart – and much more. Fig. 1 shows emulsion drop formation in a mixture of oil, water and surfactant. Fig. 2 shows the subtle "wormlike" micelle phase, and Fig. 3 shows a lamellar phase. It is interesting to note that a lamellar phase was never observed in the two-dimensional lattice-gas model (without shear). In a recent publication, we have pointed out that this is due to a theorem of Peierls, who pointed out that statistical equilibria that vary in only one of D dimensions are always unstable with respect to thermal fluctuations at any positive temperature for $D = 2$, but may be stable below a finite temperature for $D = 3$.
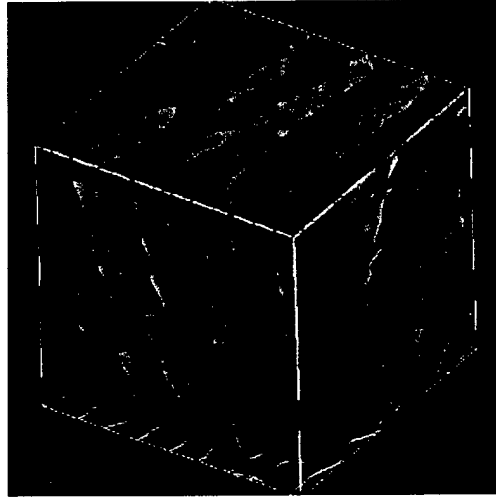
Figure 3: Lamellar phase in 3D lattice-gas model

In addition, we developed a lattice Boltzmann model of amphiphilic fluids [17], which can be run in either two or three dimensions. The model is based on the Shan-Chen paradigm [19] for adding molecular interactions to a lattice Boltzmann model. This model exhibits droplet and lamellar phases in two spatial dimensions, and these are shown in Figs. 4 and 5, respectively. Since lattice Boltzmann methods lack kinetic fluctuations, they are not subject to the above-mentioned Peierls instability, and presumably this is why they can exhibit lamellae in two dimensions.

Finally, we have applied these methods to problems of porous flow and pollution remediation [20]. Fig. 6 shows the forced flow of two immiscible fluids in a porous medium, with and without the presence of amphiphile in the invading species. It can be seen that the interface is more effectively broken up in the presence of amphiphile, resulting in dramatically different flow properties. This effect is important in the removal of hydrophobic pollutants by in situ remediation methods.

2.2 Entropic Lattice Boltzmann Models

As noted in the Introduction, lattice BGK methods lack an H-theorem, and are plagued by a variety of ill-understood numerical instabilities. In recent work, we have demonstrated a generalization of the BGK technique that makes it possible to reintroduce an H-theorem in many cases. In work begun during the period of this grant, we formulated a general program for the construction of "entropically stabilized" lattice Boltzmann models, and illustrated its application to several example problems. The expected time of publication of this work will be in early 2000 [21].

The crux of the idea is to encourage the model builder to specify an appropriate H function (Lyapunov function) for the model, rather than try to blindly dictate an equilibrium state, as is done for BGK models. Of course, specifying a form for H determines the equilibrium distribution, but it also governs the *approach* to this equilibrium. It can therefore be used to control the stability properties of the model. It should be emphasized that the presence of a Lyapunov function guarantees the *nonlinear* stability of the model, which is a much stronger condition than linear stability.

We showed that collision operators that are constructed to increase H defined in this way are similar in form to the lattice BGK collision operators, except that their relaxation parameter may depend on the current state. As a result, the transport coefficients may have a certain minimum value in models of this type but these minimum values are often actually zero. This would seem to make possible the construction of fully explicit, perfectly conservative, absolutely stable algorithms with arbitrarily small transport coefficients. In fact, we showed that the ultimate limitation to the application of these algorithms for very small transport coefficients come from considerations of accuracy, rather than stability.

Fig. 7 shows the decay of the amplitude of an initially sinusoidal density profile in a simple entropic
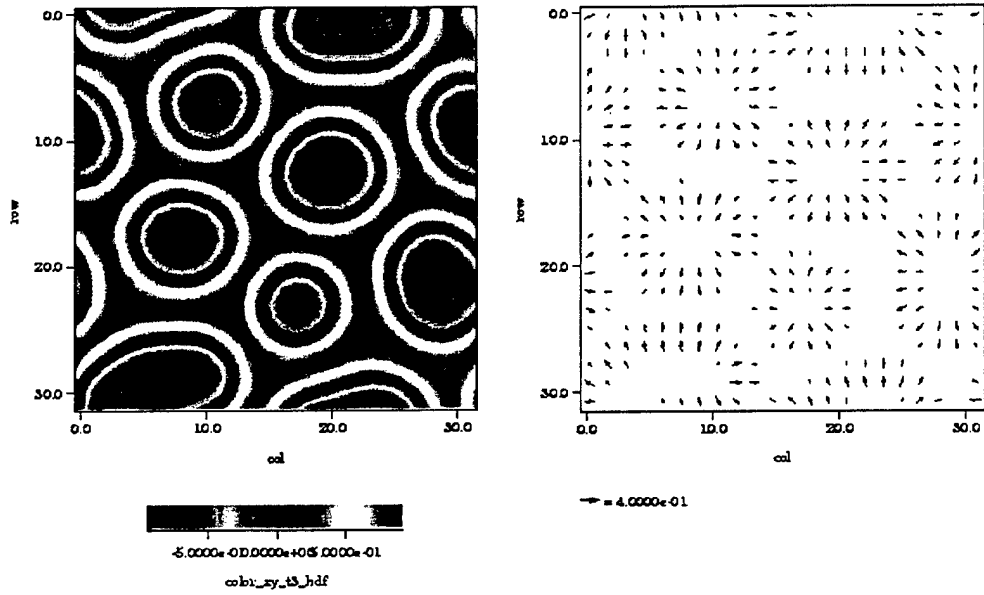
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Figure 4: Two-dimensional domain growth in a ternary (oil-water-surfactant) fluid. Colour (oil-water, left) and amphiphile director (right) distributions are both shown at lattice timestep $t = 16000$
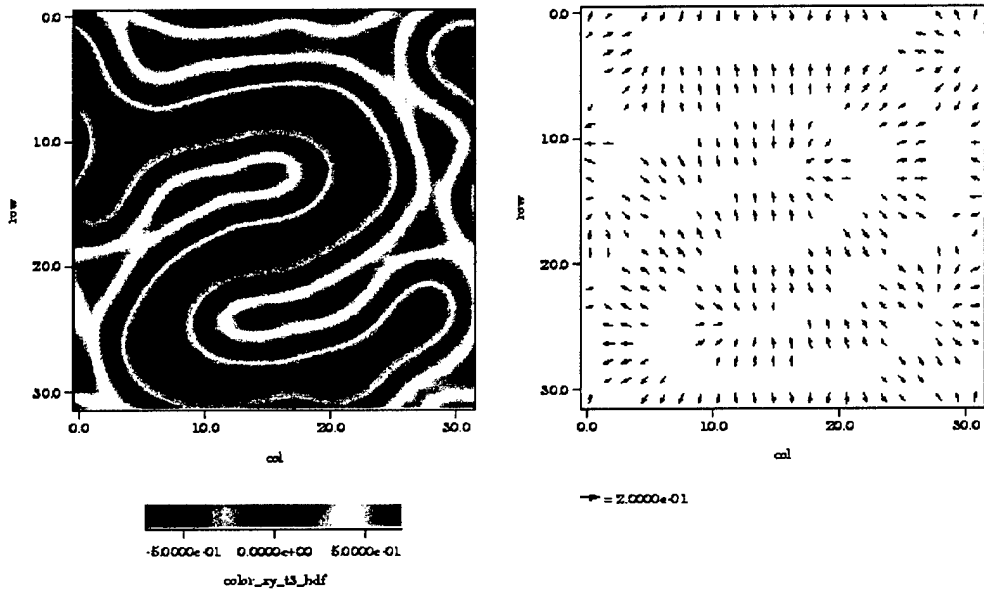

Figure 5: Formation of a lamellar phase in a ternary oil-water surfactant lattice Boltzmann fluid. Colour (left) and amphiphile (right) distribution are shown, both at lattice timestep $t = 20000$
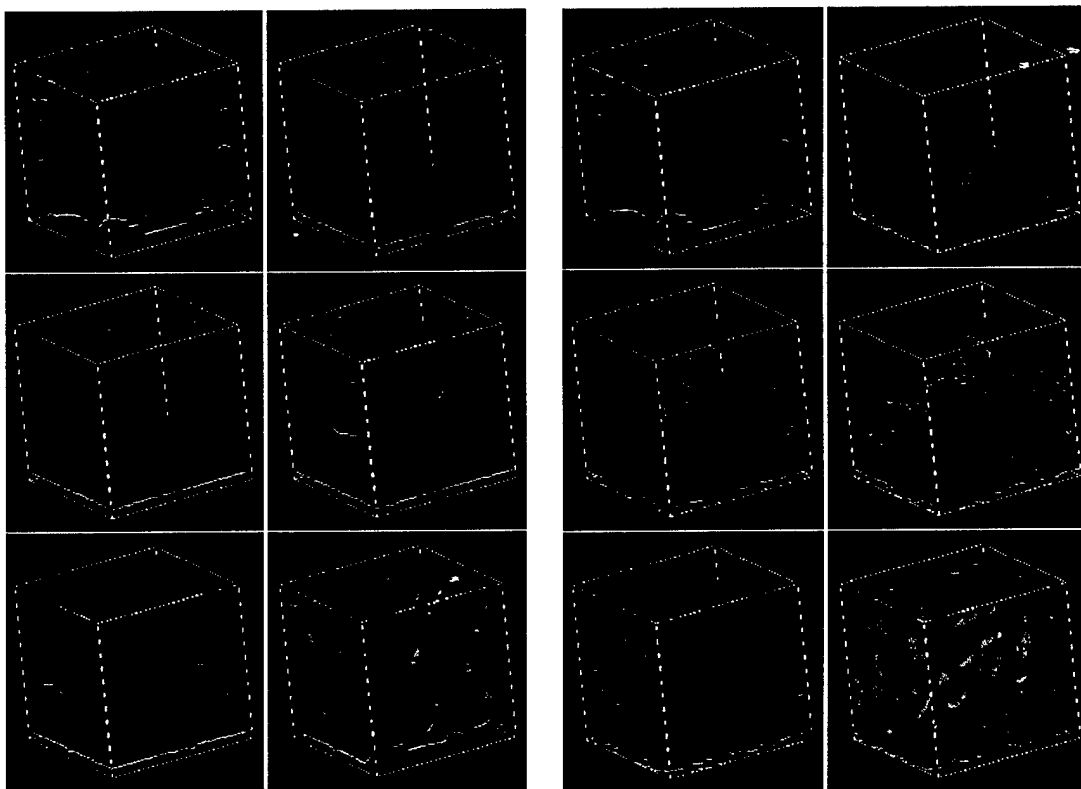
Figure 6: Flow of immiscible fluid through porous medium, without (left) and with (right) amphiphile. Note that the presence of amphiphile breaks up the interface, substantially altering the character of the flow.
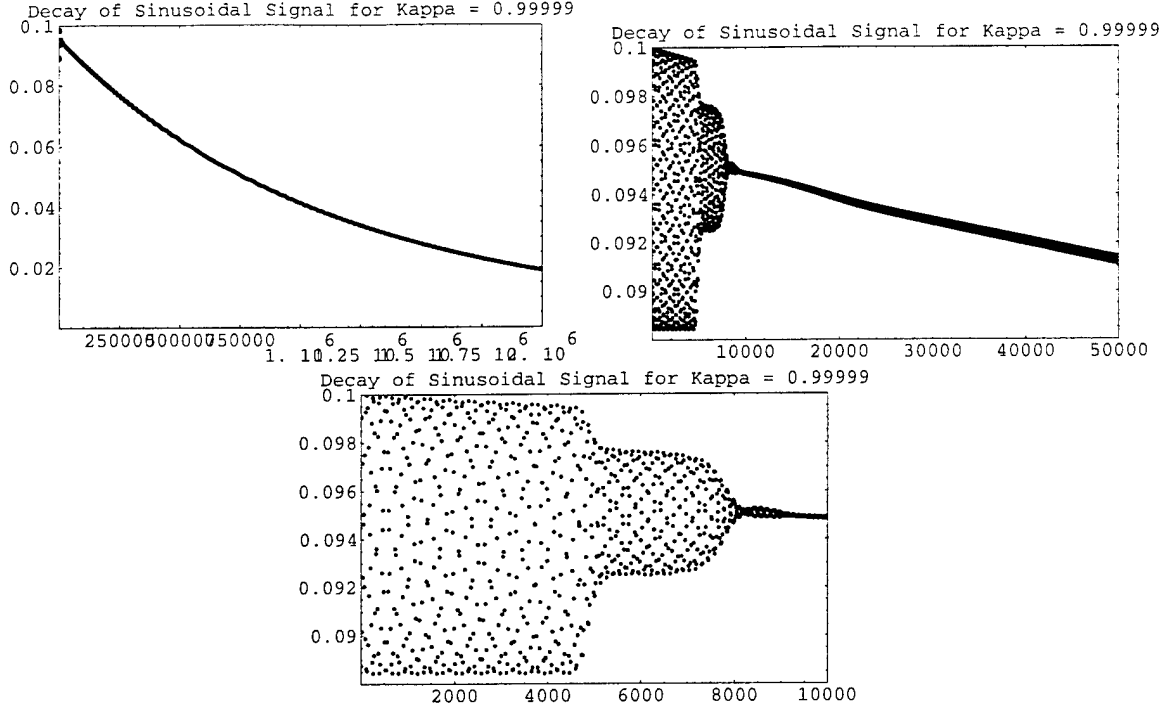
Figure 7: **Decay of sinusoidal density profile** for $\kappa = 0.99999$

lattice Boltzmann model of diffusion. This decay rate can be used to infer the diffusivity of the model, and this is compared against the corresponding theoretical value in Table 1. The parameter κ is related (in a somewhat complicated fashion – see the reference [21] for details) to the factor by which the Lyapunov function changes due to a given collision. When it is equal to unity, the Lyapunov function does not change at all, and the diffusivity vanishes; this is the marginally stable situation. Agreement between theory and numerical experiment is good until κ is extremely close to unity, so the diffusivity is extremely small, and the time required for decay of kinetic modes is not well separated from the bulk modes of interest. This gives rise to the "ringing" exhibited in Fig. 8. Nonetheless, the method is very promising because if viscosities could likewise be made this small, very high Reynolds number simulations would be possible.

2.3 Quantum Lattice Models

Quantum Lattice-Gas Automata (QLGA) is a new quantum computing paradigm, motivated by lattice-fluid models. To the extent that the LGA and LB methods can be thought of as discrete bits and real-valued
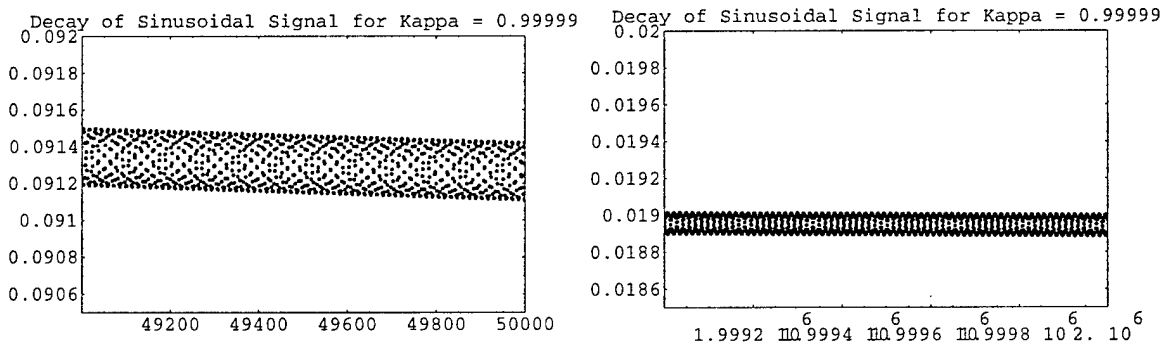
Figure 8: **Decay of sinusoidal density profile** for $\kappa = 0.99999$

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κ	D_{theory}	D_{meas}
0.9	1.852×10^{-2}	1.75364×10^{-2}
0.99	1.684×10^{-3}	1.67419×10^{-3}
0.999	1.668×10^{-4}	1.66674×10^{-4}
0.9999	1.667×10^{-5}	1.66198×10^{-5}
0.99999	1.667×10^{-6}	2.28751×10^{-6}

Table 1: **Theoretical and measured values of the diffusivity** for various values of κ.

quantities moving about on a grid, respectively, then a QLGA for a single quantum particle can be thought of as complex amplitudes doing likewise and colliding according to unitary transformations at each site. Just as the real-valued quantities of the LB method represent occupation probabilities, so do the squares of the moduli of the complex amplitudes of a QLGA. As these amplitudes move about and collide on the spatial grid, they can *interfere* with each other, giving rise to behavior that is not possible with ordinary lattice-gas automata.

Whereas an LGA with N bits can be in any one of 2^N distinct states, a QLGA can be in a complex superposition of *all* of those 2^N states – although conservation of mass (and momentum if appropriate) restricts the evolution to particular sectors of the full Hilbert space. It follows that in order to consider QLGA with more than a single particle, it is necessary to add dimensions to the configuration space for each additional particle. As noted in the introduction, this becomes rapidly intractable on any classical computer, but poses no extra problem for a quantum computer [9, 10, 11, 12]. Indeed, QLGA can be regarded as a novel paradigm for computational physics on quantum computers.

The Space Vehicles Directorate at AFRL is currently engaged in a program of realizing quantum computation using nuclear magnetic resonance (NMR) apparatus. The program's collaborators also include researchers at the M.I.T. Francis Bitter Magnet Laboratory. The NMR apparatus used is very nearly "off the shelf"; it required very little modification from those used for medical imagery. The idea is that, by placing certain organic molecules in a strong magnetic field, one can control the spin states of various nuclear spins using radio frequency. The nuclear spins are coupled by the electronic structure of the molecule. Because the NMR sample contains order 10^{18} molecules, the measured signal effectively averages over these, yielding a high signal-to-noise ratio. (It is to be emphasized, however, that only spins within the same molecule enter into a single computation.) The apparatus is able to localize subsets of the molecules according to their spatial position by using field gradients. To date, a universal quantum gate with three quantum bits has been achieved in this way at M.I.T.; up to seven uncoupled quantum bits have been achieved at the Los Alamos National Laboratory.

Since Schrödinger's equation can be related, via a well-known mathematical transformation, to Euler's equation for inviscid fluid flow, our investigations with the AFRL group have centered on whether or not it would be possible to use an array of NMR machines for very fast – and very high Reynolds number – fluid flow simulations. Towards this end, we have constructed a (classical) computer simulation of a one-dimensional quantum lattice gas with a conserved mass, momentum and energy. The code works by diagonalizing the discrete quantum system, and so it can be used only on small lattices. We are able to simulate this system under a variety of conditions, however, including the periodic performing of measurements or partial measurements during the simulation. Our goal is to simulate systems of various sizes in order to discern the scaling behavior of the system in the hydrodynamic limit.

As of the end of the grant reporting period, this work is ongoing. We expect that it will result in a publication in the middle of calendar year 2000 [22].

3 Conclusions

We have described the program of activity of the lattice-gas research collaboration between the Boston University Center for Computational Science and the Space Vehicles Directorate of AFRL (under AFOSR task 2304CP). This collaboration has centered on three major areas of study: (i) lattice-fluid models for droplet formation, (ii) entropic lattice Boltzmann models, and (iii) quantum lattice-gas automata. We have provided a detailed account of the principal new results in all three of these areas. Nine publications have

resulted from this effort, as well as the sponsorship of the Seventh International Conference on Discrete Models for Fluid Mechanics, and the preparation of the proceedings of that meeting as a special issue of the *International Journal of Modern Physics C*.

References

[1] U. Frisch, B. Hasslacher, and Y. Pomeau, *Phys. Rev. Lett.* **56** 1505 (1986).

[2] S. Wolfram, *J. Stat. Phys.* **45**, 471 (1986).

[3] U. Frisch et al., *Complex Syst.* **1**, 648 (1987).

[4] D.H. Rothman and S. Zaleski, *Lattice-Gas Automata: Simple Models of Complex Hydrodynamics*, (Cambridge University Press, 1997).

[5] S. Succi, R. Benzi, F. Higuera, *Physica D* **47** (1991) 219-230.

[6] R. Benzi, S. Succi, and M. Vergassola *Phys. Rep.*, **222** 145 (1992).

[7] E. Gross, D. Bhatnager, M. Krook, *Phys. Rev.* **94** (1954) 511.

[8] Y.-H. Qian, D. d'Humières, P. Lallemand, *Europhys. Lett.* **17** (1992) 479-484.

[9] D. Meyer, *J. Stat. Phys.* **85** (1996) 551-574.

[10] B.M. Boghosian, W. Taylor, *Phys. Rev. E* **56** (to appear, 1997).

[11] B.M. Boghosian, W. Taylor, in *Proc. PhysComp '96* (submitted, 1996).

[12] B.M. Boghosian, W. Taylor, *Int. J. Mod. Phys. C* **8** (1997) 705.

[13] R. Feynman, *Int. J. Theor. Phys.* **21** (1982) 467-488; *Found. Phys.* **16** (1986) 507-531.

[14] J.-B. Maillet, V. Lachet, P.V. Coveney, preprint cond-mat/9911013, Department of Chemistry, Queen Mary and Westfield College, University of London (1999).

[15] B.M. Boghosian, P.V. Coveney, A.N. Emerton, *Proc. Roy. Soc. A* **452** (1996) 1221.

[16] B.M. Boghosian, P.V. Coveney, P.J. Love, *Proc. Roy. Soc. Lon.* (to appear, 1999).

[17] H. Chen, B.M. Boghosian, P.V. Coveney, preprint submitted to *Proc. Roy. Soc.* (1999).

[18] C. Appert, J.F. Olson, D.H. Rothman, S. Zaleski, *J. Stat. Phys.* **81** (1995) 181-197.

[19] X. Shan, H. Chen, *Phys. Rev. E* **47** (1993) 1815-1819.

[20] P.V. Coveney, J.-B. Maillet, J.L. Wilson, P.W. Fowler, O. Al-Mushadani, B.M. Boghosian, *Int. J. Mod. Phys. C* **9** (1998) 1479-1490.

[21] B.M. Boghosian, J. Yepez, A. Wagner, P.V. Coveney, "Entropic Lattice Boltzmann Models," Boston University Center for Computational Science preprint (2000).

[22] B.M. Boghosian, J. Yepez, in preparation.

A Publications

The following nine publications coauthored by Bruce M. Boghosian acknowledged the support of this grant:

1. B.M. Boghosian, P.V. Coveney, "A Particulate Basis for an Immiscible Lattice-Gas Model," *Comp. Phys. Comm.* (to appear, 1999).

2. H. Chen, B.M. Boghosian, P.V. Coveney, "A Ternary Lattice Boltzmann Model for Amphiphilic Fluids," submitted to *Phys. Rev. E* (1999).

3. B.M. Boghosian, P.V. Coveney, P.J. Love, "A Three-Dimensional Lattice-Gas Model for Amphiphilic Fluid Dynamics," *Proc. Roy. Soc. Lon.* (to appear, 1999).

4. B.M. Boghosian, "A Generalization of Metropolis and Heat-Bath Sampling for Monte Carlo Simulations," *Phys. Rev. E* **60** (1999) 1189-1194.

5. B.M. Boghosian, "Navier-Stokes Equations for Generalized Thermostatistics," *Braz. J. Phys.* **29** (1999) 91-107.

6. B.M. Boghosian and P.V. Coveney, "Inverse Chapman-Enskog Derivation of the Thermohydrodynamic Lattice-BGK Model," *Int. J. Mod. Phys.* C **9** (1998) 1231-1246.

7. P.V. Coveney, J.-B. Maillet, J.L. Wilson, P.W. Fowler, O. Al-Mushadani and B.M. Boghosian, "Lattice Gas Simulations of Ternary Amphiphilic Fluid Flow in Porous Media," *Int. J. Mod. Phys.* C **9** (1998) 1479-1490.

8. F.W.J. Weig, P.V. Coveney and B.M. Boghosian, "Lattice-Gas Simulations of Minority-Phase Domain Growth in Binary Immiscible and Ternary Amphiphilic Fluid," *Phys. Rev. E* **56** (1997) 6877-6888.

9. A.N. Emerton, P.V. Coveney and B.M. Boghosian, "Applications of a Lattice-Gas Automaton Model for Amphiphilic Systems," *Physica* A **239** (1997) 373-381.

B Invited Talks and Presentations

The following invited talks and presentations by Bruce M. Boghosian were related to the topic of this grant proposal, and were presented during the time period of the grant:

1. Speaker, Silicon Graphics Scientific Visualization Seminar, Boston University. Boston, Massachusetts (31 March 1999).

2. Speaker, Conference on Computational Physics '99, American Physical Society Centennial Meeting, Atlanta, Georgia (25 March 1999).

3. Session chair, Conference on Computational Physics '99, American Physical Society Centennial Meeting, Atlanta, Georgia (25 March 1999).

4. Colloquium speaker, Department of Applied Mathematics, Brown University, Providence, Rhode Island (18 March 1999).

5. Colloquium speaker, Department of Applied Science, University of California, Davis (4 March, 1999).

6. Colloquium speaker, Department of Physics, Brandeis University, Waltham, Massachusetts (24 November 1998).

7. Seminar speaker, Air Force Research Laboratory, Space Vehicles Directorate, Hanscom AFB, Massachusetts (16 September, 1998).

8. Speaker, Conference on Computational Physics (CCP98), Granada, Spain (2-5 September, 1998).

9. Speaker, Seventh International Conference on the Discrete Simulation of Fluids, Oxford, England (14-18 July, 1998).

10. Speaker, Workshop on Computational Tools for Multiphase/Multicomponent Polymer Materials, Center for Theoretical and Computational Materials Science, National Institute of Standards and Technology (20-21 May, 1998).

11. Colloquium speaker, Department of Physics, Swarthmore College, Swarthmore, Pennsylvania (17 April, 1998).

12. Colloquium speaker, Department of Physics, University of Massachusetts, Amherst, Massachusetts (4 February, 1998).

C Proceedings of the Seventh International Conference on Discrete Models for Fluid Mechanics

This is the table of contents of the Proceedings of the Seventh International Conference on Discrete Models for Fluid Mechanics. These proceedings, edited by Bruce M. Boghosian, have been published as a special issue (Vol. 9, No. 8, December, 1998) of the *International Journal of Modern Physics C.*

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